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# CALCULATION OF ESSENTIAL CHARACTERISTICS FOR EM SIGNAL TRANSPORTING ALONG LINEAR NANO-SCALE Ag/Au/Cu-WAVEGUIDES IN $SIO_2$

*Abstract – Propagation of surface dipole oscillations along a linear chain composed of spherical nanoparticles of noble metals is considered. It was calculated the EM signal longitudinal group velocities $V_{gr,Z}$ and the effective lengths $L_z$ of the signal "run" along nano-scale 1D-waveguides which are composed of Ag/Au/Cu nanospheres at different temperatures and at the most frequently used parameters of such waveguides placed into $SiO_2$ : the values are in good agreement with experimental data. The fact can be used to transfer information over relatively large distances: $L_z$ > 2 μm, i.e. over the distances which exceed 200 periods of the nanoscale linear structure.*

*Keywords: surface dipole oscillations, metal nanoparticles, nanoscale waveguides.*

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**РАСЧЕТ ГРУППОВОЙ СКОРОСТИ РАСПРОСТРАНЕНИЯ ЭМ СИГНАЛА ВДОЛЬ НАНОМАСТАБНЫХ Ag/Au/Cu-ВОЛНОВОДОВ, ПОГРУЖЕННЫХ В $SIO_2$**

*Рассмотрено распространение поверхностных дипольных колебаний вдоль линейной цепочки, составленной из сферических наночастиц благородных металлов. Вычислены продольные скорости $V_{gr,Z}$ прохождения ЭМ сигнала и эффективные длины $L_z$ «пробега» сигнала вдоль наноразмерных Ag/Au/Cu-волноводов при различных температурах и наиболее часто используемых параметрах такого рода волноводов, погруженных в $SiO_2$ : полученные расчеты находятся в хорошем согласии с экспериментом. Этот факт может быть использован для передачи информации на сравнительно большие расстояния: $L_z$ > 2 мкм, т.е. на расстояния, превышающие 200 периодов такой линейной структуры.*

*Ключевые слова: поверхностные дипольные колебания, металлические наночастицы, наноразмерный волновод.*

## Introduction

Recent experimental and theoretical studies of plasma oscillations in metallic nanoparticles produce various techniques which can be used for signal transporting, and these phenomena are also of great practical importance [1], because such systems can be assigned to nanoscale waveguides which are possible basis for development of new generation of optical communication systems [2, 3]. One-dimensional ordered arrays of noble metal (Au, Ag, Cu) spherical nanoparticles are successfully considered as waveguides that are suitable for these purposes. It is well established that the nanoparticles of noble metals support plasmon resonances within a wide frequency range (UV $\rightarrow$ visible $\rightarrow$ near IR) [2-5].

Most frequently one investigates the properties of plasma 1D-waveguides consisting of noble metal nanospheres with a diameter of 40-50 nm or of similar size [2, 3, 6]. Now it is the well known fact, that propagating plasma oscillations which arise in the "chain" due to the external electromagnetic wave source (generator), do not decay eventually, and the greatest amplitudes of the plasma waves appear at the resonance frequencies [5-8].

Since the signal transporting issue along nanoscale waveguides placed in different dielectric host is very important, is necessary to know a lot of the technological parameters of these devices within a wide range of temperatures.

The aim of this work was to establish dependences of some basic parameters of the signal transportation along the described nanoscale waveguides in the form of a linear array ("nano-chains") which are composed of metallic nanospheres and they are merged into a dielectric medium – $SiO_2$.

## On plasma oscillations waveguiding: Theory

Consider an infinite chain composed of noble metal nanoparticles of spherical shape of radius $a$ and the chain is hosted in a dielectric medium with dielectric constant of $\varepsilon_h$ . We suppose that the nanospheres are arranged along an axis $Z$ at an equal distance of $d > 2a$ from each other (i.e., their centers are spaced at equal distances from each other, as it shown in Fig. 1). Let the origin of coordinates is located at the center of one of the particles, for example at the nanosphere with index $l = 0$ . Further suppose that there is an external source of electric field, which is located on one of the particles of the nanochain, for example, on the particle with index $l = 0$ . At the center of the particle with $l = 0$ this electric field produces a point dipole moment which, in its turn, will also radiate a certain electric field.

Let the intensity of the radiated electric field at any point of the axis $Z$ at any given time $t$ is equal to $\vec{E}_0(0;z;t)$ , in this case $\vec{E}_0(0;z;t) = \vec{E}_0(0;-z;t)$ .

Then projection of the considered electric field intensity onto the coordinate axe $Z$ at each $l$ -th node of

the chain, where are located metal nanoparticles, will be determined by the following relations: $\vec{E}_{0z}(0;ld;t) = \lim\limits_{z \to ld} E_{0z}(0;z;t)$.

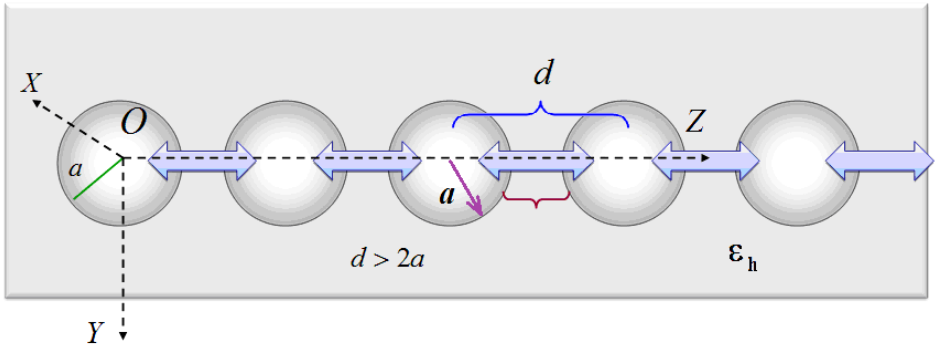


**Fig. 1 : a schematic representation of the linear array of metallic nanospheres of radius *a*, which are spaced by a distance of *d* and are placed in $SiO_2$**

It means that at the center of each metal nanoparticles (see [6, p. 124322, Eq. (27)]) it will arise additional dipole moments, committing with time compelled transverse and longitudinal vibrations.

From a theoretical viewpoint (see [4-6]), the dipole moment $\vec{D}(\vec{R},t)$ located at the point $\vec{R}$ radiates an electric field with its intensity at a point $(\vec{R} + \vec{R}_0)$ of:

$$\vec{E}(\vec{R};\vec{R}_0;t) = \frac{1}{\varepsilon_h}\left(-\frac{1}{R_0^3} - \frac{1}{R_0^2}\frac{1}{V_h}\frac{\partial}{\partial t} - \frac{1}{R_0}\frac{1}{V_h^2}\frac{\partial^2}{\partial t^2}\right)\times$$

$$\times \vec{D}\left(\vec{R};t - R_0/V_h\right) + \frac{1}{\varepsilon_h}\left(\frac{3}{R_0^3} + \frac{3}{R_0^2}\frac{1}{V_h}\frac{\partial}{\partial t} + \frac{1}{R_0}\frac{1}{V_h^2}\frac{\partial^2}{\partial t^2}\right)\vec{n}_0 \cdot \left(\vec{n}_0 \cdot \vec{D}\left(\vec{R};t - R_0/V_h\right)\right),$$

where $\vec{n}_0 = \vec{R}_0/R_0$, $V_h = c/\sqrt{\varepsilon_h}$.

Plasma oscillations arising on the particle with index $l$ also emit electromagnetic field, which is accompanied by power emitted by the influence of the field on the conduction electrons of the particle with index $l$ (it is about Lorentz force, see [4, 5]). The presence of this force is equivalent to the presence of an external electric field effective, the source of which is located in the center of the particle with index $l$, and the intensity of this field is given by the expression (see [4-6]):

$$\vec{E}_L(ld,0,t) = \frac{2e\sqrt{\varepsilon_h}}{3c^3\varepsilon_h}\frac{\partial^3 \vec{D}(ld,t)}{\partial t^3} = \frac{2}{3d^3\varepsilon_h}\left(\frac{d}{V_h}\right)^3 \frac{\partial^3 \vec{D}(ld,t)}{\partial t^3}.$$

Thus, the equations describing the behavior of the dipole moment $\vec{D}_z(ld,t)$ along the longitudinal direction ($Z$ axis) of the particle with index $l$ are of the form (see [6, p. 124322, see Eq. (28-29)]):

$$\frac{\partial^2 D_z(ld,t)}{\partial t^2} + \frac{2}{\tau_0}\frac{\partial D_z(ld,t)}{\partial t} + \omega_1^2 D_z(ld,t) = \varepsilon_h a^3 \omega_1^2 \left(\sum_{\substack{m=-\infty \\ (m \neq l)}}^{+\infty} E_z(R_m, R_{ml}, t) + E_{Lz}(ld,0,t) + E_{0z}(0,ld,t)\right), \quad (1)$$

where $\tau_0 = \left(\frac{V_F}{2\lambda_b} + \frac{V_F}{2a}\right)^{-1}$ is the decay time of plasma oscillations due to their interaction with phonons of bulk metal and surface of the nanoparticles.

For the particle with index $m$ ($m \neq l$), equations (1) can be rewritten as

$$\frac{\partial^2}{\partial t^2} D_z(ld,t) + \frac{2}{\tau_0}\frac{\partial}{\partial t} D_z(ld,t) + \omega_1^2 D_z(ld,t) =$$

$$= 2\omega_1^2 \frac{a^3}{d^3}\left[\sum_{\substack{m=-\infty \\ (m \neq 0)}}^{+\infty}\left(\frac{1}{|m|^3} + \frac{d}{V_h |m|^2}\frac{\partial}{\partial t}\right) \cdot D_z\left(md + ld; t - \frac{|m|}{V_h}d\right) + \frac{d^3}{3V_h^3}\frac{\partial^3}{\partial t^3} D_z(ld;t)\right] + \varepsilon_h a^3 \omega_1^2 E_{0z}(0;ld;t).$$

Here $l \cdot d$ is the discrete variable. To solve these equations, assume that $D_z(ld,t) = \lim\limits_{z \to ld} D_z(z,t)$, where $z$ is the continuous independent variable, and functions $D_z(z,t)$ satisfy the following equations:

$$\frac{\partial^2}{\partial t^2}D_z(z,t)+\frac{2}{\tau_0}\frac{\partial}{\partial t}D_z(z,t)+\omega_1^2 D_z(z,t)=$$

$$=2\omega_1^2\frac{a^3}{d^3}\left[\sum_{\substack{m=-\infty\\(m\neq 0)}}^{+\infty}\left(\frac{1}{|m|^3}+\frac{d}{V_h|m|^2}\frac{\partial}{\partial t}\right)\cdot D_z\left(md+z;t-\frac{|m|}{V_h}d\right)+\frac{d^3}{3V_h^3}\frac{\partial^3}{\partial t^3}D_z(z;t)\right]+\varepsilon_h a^3\omega_1^2 E_{0z}(0;z;t).$$

Here: $\omega_1^2=\dfrac{\omega_p^2}{3\varepsilon_h}$ is the frequency of plasma oscillations in a medium where the nanoparticles are placed;

$\omega_p$ is the eigenfrequency of plasma oscillations of the electron gas of the nanoparticles.

Next we suppose that the external electric field is turned off at the moment of $T$.

A way to solve this DE is described in detail in [9]. Under the conditions $z=ld$ and $t>T$ the mentioned above short-term effect of external electric field on the dipole moment of the $l$-th nanospheres of the nanochain takes the form (see [9]):

$$D_z(ld,t)=\frac{\varepsilon_h a^3\omega_1^2}{\widetilde{\omega}_z'(\pi)}\frac{2\Delta k}{\exp(t/\tau_0)}\times$$

$$\times\operatorname{Im}\left[F_z(k_0,T)\frac{\sin\left(ld-t\Delta k\cdot\left.\dfrac{d\widetilde{\omega}_z'}{dk}\right|_{\pi/d}\right)}{ld-t\Delta k\cdot\left.\dfrac{d\widetilde{\omega}_z'}{dk}\right|_{\pi/d}}\right]\cdot\left[\exp\left(i\widetilde{\omega}_z'(\pi)\cdot t+ik_0ld\right)+\exp\left(i\widetilde{\omega}_z'(\pi)\cdot t-ik_0ld\right)\right], \qquad (2)$$

here we have denoted: $k_0=\Delta k=\pi/d$.

**On signal propagation along nano-waveguides: Results**

From Eq. (2) we can see that the function is a wave packet: the last factor here is so-called a "rapidly-oscillating" function, and the factor in square brackets before is the amplitude of the changing with time dipole moment of the nanoparticle with index $l$.

This maximum of the amplitude can be achieved at the moment $t_l=ld/V_{gr,Z}$, where $V_{gr,Z}=\left(\dfrac{d\widetilde{\omega}_z'(kd)}{dk}\right)\Big|_{k=\pi/d}=\dfrac{\tau_0\omega_z'(kd)}{\sqrt{(\tau_0\cdot\omega_z'(kd))^2-1}}\cdot\left.\dfrac{d\omega_z'(kd)}{dk}\right|_{k=\pi/d}$ is the group velocity of the wave packet, at which it moves along the nanochain.

The dipole moment $D_z(ld,t)$ of the particle with index $l$ after termination of external influence, i.e. at $t>T$, has the following form:

$$D_z(ld,t)=\varepsilon_h\frac{a^3\omega_1^2}{\widetilde{\omega}_z'(\pi)}(-1)^l\cdot\frac{\sin\left(\widetilde{\omega}_z'(\pi)\cdot t\right)}{\exp(t/\tau_0)}\cdot\frac{\sin\left(\pi l-\pi t\cdot V_{gr,Z}/d\right)}{\pi\cdot\left(l-t\cdot V_{gr,Z}/d\right)}\cdot\int_0^T\exp(t_1/\tau_0)E_{0z}(0;0;t_1)dt_1, \qquad (3)$$

From the eq. (3) one can see that the dipole moment of the $l$-th nanoparticle reaches its maximum value at $t=t_l=ld/V_{gr,Z}$, and the maximum value at this moment is directly proportional to the value of $\exp(-t_l/\tau_0)$. Hence the distance $L_z=V_{gr,Z}\cdot\tau_0$, on which a signal can be transmitted along a linear array of nanoparticles, may be called signal propagation "effective length" $L_z$: this distance can be regarded as an effective because of losses of signal power during its propagation at this length along considered nanoscale waveguides do not exceed 5% of its initial level [3, 9].

Some basic characteristics of nanoscale waveguides were calculated *ab initio* within theoretical viewpoints, published in [4, 7, 9]. After Fourier transformation of Eq. (3) one can get the following relation for the longitudinal group velocity $V_{gr,Z}$:

$$V_{gr,Z}=\frac{2d\cdot\omega_1^2\cdot\sum_{m=1}^{\infty}\dfrac{\sin(m\cdot kd)}{m}\cdot\left(\dfrac{\cos(m\cdot\omega_1 d/V_h)}{m}+\omega_1 d/V_h\cdot\sin(m\cdot\omega_1 d/V_h)\right)}{\left(\dfrac{d}{a}\right)^3\cdot\sqrt{\omega_1^2\cdot\left[1-4\cdot\left(\dfrac{a}{d}\right)^3\cdot\sum_{m=1}^{\infty}\dfrac{\cos(m\cdot kd)}{m^2}\cdot\left(\dfrac{\cos(m\cdot\omega_1 d/V_h)}{m}+\omega_1 d/V_h\cdot\sin(m\cdot\omega_1 d/V_h)\right)\right]-\dfrac{1}{\tau_0^2}}}$$

The results of calculations are presented in the Table 1. The presented characteristics of the waveguides

were calculated at resonant frequencies for the given array configurations, and also for the parameters listed below – for a given temperature, the different radii $a$ and the distances $d$ between the centers of the particles.

Table 1

**The values of the longitudinal group velocities $V_{gr,Z}$ and signal propagation lengths $L_z$ for nanoscale Ag/Au/Cu-waveguides hosted in $SiO_2$ ($T$ = 300 K)**:

| radius $a$, nm | *the signal group velocity* $V_{gr,Z}$ *at* ***d*/*a*=2,5** | | | *the signal propagation effective length* $L_z$, μm | | |
|---|---|---|---|---|---|---|
| | $V_{gr,Z}$, (Ag) | $V_{gr,Z}$, (Au) | $V_{gr,Z}$, (Cu) | $L_z$, (Ag) | $L_z$, (Au) | $L_z$, (Cu) |
| 5 | 0,025·***c*** | 0,025·***c*** | 0,031·***c*** | 0,050 | 0,048 | 0,052 |
| 15 | 0,099·***c*** | 0,099·***c*** | 0,141·***c*** | 0,493 | 0,455 | 0,578 |
| 25 | 0,363·***c*** | 0,355·***c*** | 0,183·***c*** | 2,631 | 2,283 | 1,051 |
| 35 | 0,077·***c*** | 0,075·***c*** | | 0,695 | 0,579 | |

| radius $a$, nm | *the signal group velocity* $V_{gr,Z}$ *at* ***d*/*a*=3,0** | | | *the signal propagation effective length* $L_z$, μm | | |
|---|---|---|---|---|---|---|
| | $V_{gr,Z}$, (Ag) | $V_{gr,Z}$, (Au) | $V_{gr,Z}$, (Cu) | $L_z$, (Ag) | $L_z$, (Au) | $L_z$, (Cu) |
| 5 | 0,018·***c*** | 0,018·***c*** | 0,022·***c*** | 0,035 | 0,034 | 0,037 |
| 15 | 0,082·***c*** | 0,083·***c*** | 0,143·***c*** | 0,412 | 0,381 | 0,586 |
| 25 | 0,103·***c*** | 0,102·***c*** | 0,031·***c*** | 0,748 | 0,653 | 0,176 |

| radius $a$, nm | *the signal group velocity* $V_{gr,Z}$ *at* ***d*/*a*=3,5** | | | *the signal propagation effective length* $L_z$, μm | | |
|---|---|---|---|---|---|---|
| | $V_{gr,Z}$, (Ag) | $V_{gr,Z}$, (Au) | $V_{gr,Z}$, (Cu) | $L_z$, (Ag) | $L_z$, (Au) | $L_z$, (Cu) |
| 5 | 0,013·***c*** | 0,013·***c*** | 0,017·***c*** | 0,026 | 0,025 | 0,028 |
| 15 | 0,080·***c*** | 0,081·***c*** | 0,122·***c*** | 0,402 | 0,374 | 0,498 |
| 25 | 0,027·***c*** | 0,026·***c*** | | 0,195 | 0,167 | |

Remarks: here ***c*** – the speed of light in vacuum; for presented in the Table #1 calculations it was taken the following basic conditions: temperature = 27 °C; supposed dielectric medium is $SiO_2$.

Carried out calculations show that for all three materials from which the waveguides are made of, there are sharp peaks (spikes) of longitudinal group velocities of signal transmission, and the growth of this ratio $d/a$ shifts the peak considerably towards nanospheres with smaller diameter (see Fig. 2). And according to obtained results this dependence of the longitudinal group velocity for each of the investigated material is strictly individual.

The noticeable difference in dependence of the longitudinal group velocity on the radius of nanospheres and the distance between of their centers, as the author believes, is caused by the differences in the electronic structure of atoms of matter the chain was made of.

### On the temperature dependence of signal group velocity

To answer the question of the stability of the signal transportation parameters as it runs along nanoscale waveguides when the ambient temperature changes, the corresponding calculations were performed. In forming the "temperature effect" on the signal running along nano-waveguides one of the main roles is played by a specific time $\tau_0$ – the decay time of plasma oscillations (see Eq. (1)).

Obtained dependence concerning to group velocities proved to be very weak (see Fig. 3): below we can see the situation for Ag nanochains (in $SiO_2$) within the temperature range from –10 °C to 300 °C. A similar pattern can be seen for other noble metals placed in the host.

### Summary

In this paper, the subject of the study was the spread of EM signal along a 1D-array which is composed of noble metal spherical nanoparticles. If external electric field source will be placed amongst such ensemble of nanoparticles, and one of the particles would be affected by a short pulse, then in this linear array the pulse will cause additionally arising of dipole waves with a frequency lower than the plasma one. As it was shown, under certain parameters of described nanoscale waveguides undamped dipole oscillations may occur in the form of a wave packet. The fact was confirmed experimentally [1, 3, 7, 8] and it can be used to transfer information over

relatively large distances: $L_{chain}$ > 2 μm, i.e. over the distances which exceed 200 periods of the nanoscale linear structure.

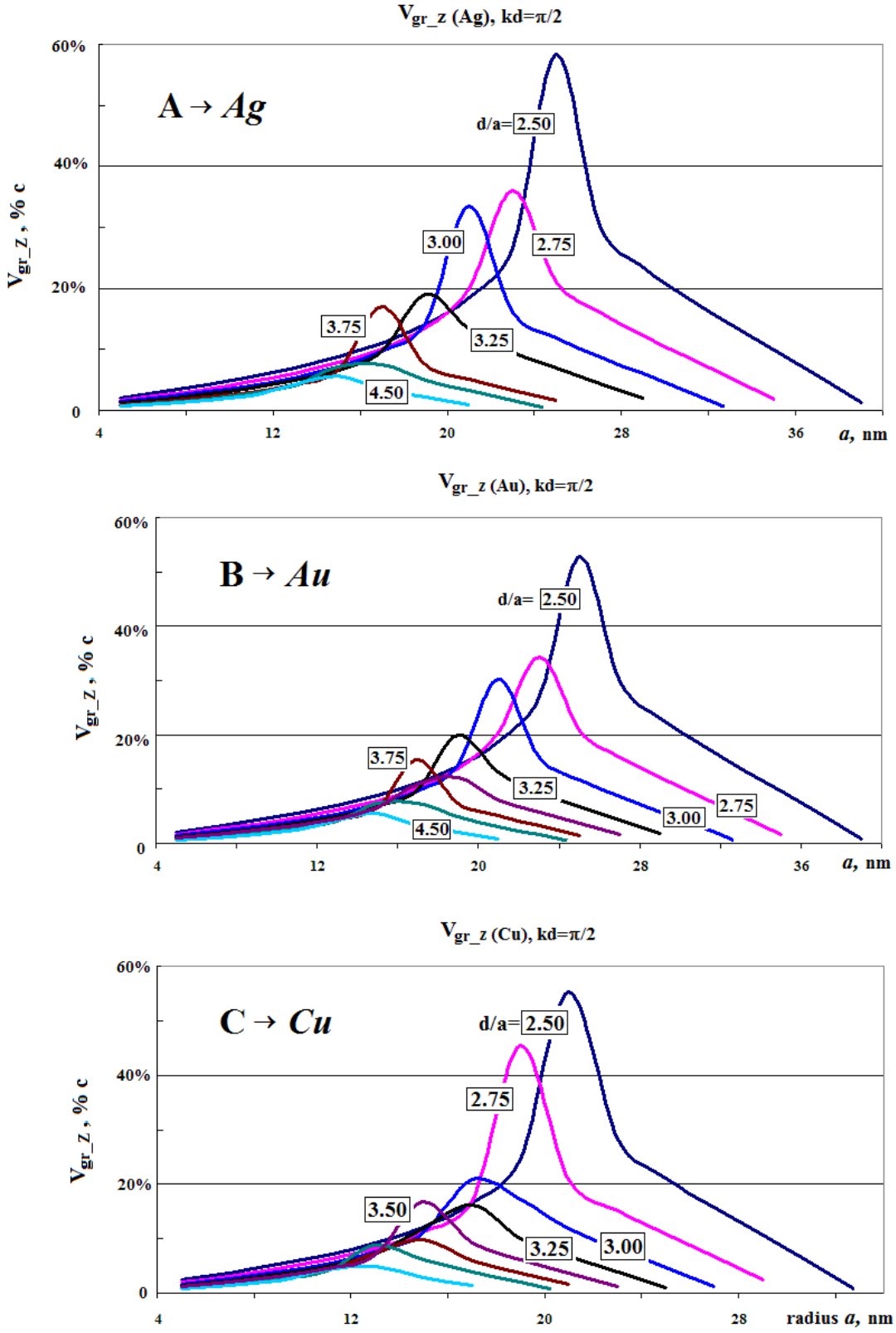


**Fig. 2 : the variation of the longitudinal group velocity $V_{gr,Z}$ of EM signal propagation along a *silver* nanochain (A), and a *gold* one (B), and a *copper* one (C), influenced by the geometric parameters[1] of the 1D-array hosted in $SiO_2$ (T=300 K)**

[1] different radii ***a*** of metallic nanospheres and different distances ***d*** between them (the ***d*/*a*** ratio)

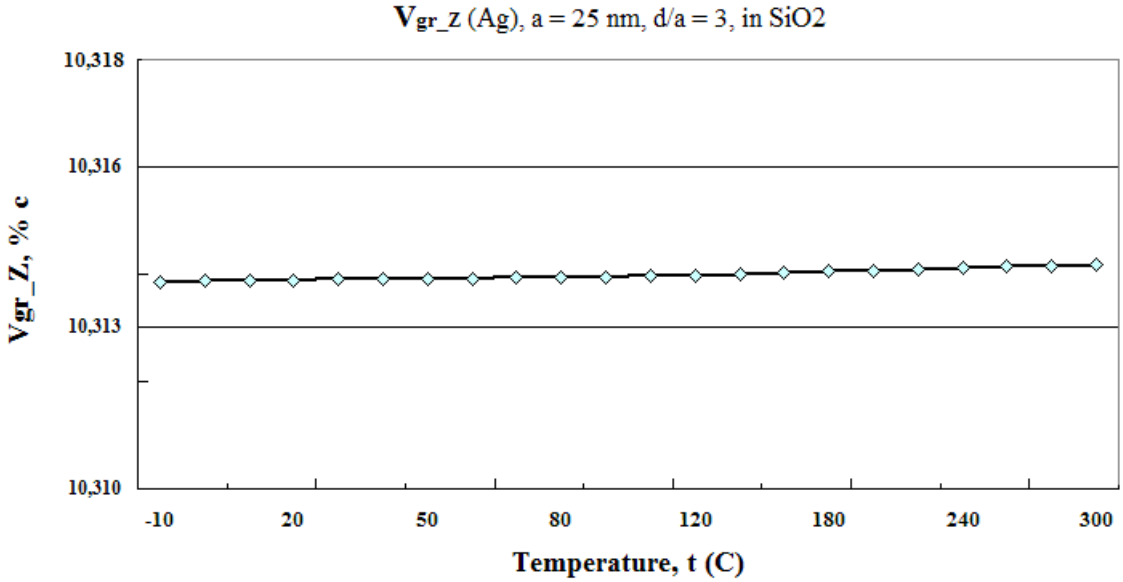


**Fig. 3 : The temperature dependence of the longitudinal group velocity of EM transmission along nanoscale *silver* waveguides composed of nanospheres with the radius *a* =25 nm (*d*/*a* =3) in $SiO_2$**

It was calculated the longitudinal group velocity $V_{gr,Z}$ of the signal running along the considered nano-scale Ag/Au/Cu-waveguides and the "effective" length of the signal propagation $L_z$ along the linear array of nanoparticles at the wide range of temperatures (placed into supposed dielectric medium of $SiO_2$). The presented results clearly show the significant dependence of the longitudinal group velocity $V_{gr,Z}$ of the signal running along one-dimensional arrays of nanoparticles (as well as the "effective" length $L_z$) on the geometric characteristics of the waveguides (see Table 1).

It should also be noted the obvious temperature-stable characteristics of signal running along the described nanowaveguides.

One can see the perspective use of the described nanoscale waveguides: 1) light energy conversion inside semiconductor photodiode systems with active nano-modified surface; and/or 2) transportation of EM energy and information within respective nano-optical devices.

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